

Unquenched domain wall quarks with multi-bosons

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Abstract

The numerical simulation of domain wall quarks with the two-step multi-boson (TSMB) algorithm is considered. The inclusion of single quark flavours, as required for strange quarks, is discussed. The usage of computer memory can be kept relatively low, independently of the order of polynomial approximations. Tests are performed with two flavours ($N_f = 2$) of degenerate quarks near the $N_t = 4$ thermodynamical cross over.

1 Introduction

Domain wall fermions [1, 2, 3] offer the possibility of improving chiral symmetry of lattice discretizations for fermionic theories by tuning the action parameters in an extra (fifth) dimension. It can be shown [4] that in the limit of vanishing lattice spacing in the fifth dimension the domain wall formulation is equivalent to the overlap formulation [5] which fulfills the Ginsparg-Wilson relation for lattice chiral symmetry [6, 7]. The price of the chiral symmetry at non-zero lattice spacing is the extra dimension enlarging the number of degrees of freedom and, from a technical point of view, the extensions of the fermion matrix. It is an interesting question how much numerical simulations with light domain wall quarks become slower than, say, with “unimproved” Wilson fermions.

Up to now unquenched domain wall fermions have been treated either by the Hybrid Monte Carlo [8] or, in case of an odd number of fermionic flavours, by the Hybrid Molecular Dynamics R-algorithm [9]. (For a few examples of these simulations see, for instance, [10, 11, 12, 13]. For a recent review see [14].) In the present paper the application of the two-step multi-boson (TSMB) algorithm [15] for domain wall fermion simulations is

considered. This algorithm is applicable for any number of fermion flavours and has a tolerable slowing down towards light fermions.

The plan of this paper is as follows: in the next Section the lattice action for two degenerate domain wall quarks is formulated. In Section 3 the TSMB algorithm is briefly recapitulated and the generalization to the case of an odd number of domain wall fermion flavours is discussed. In Section 4 the results of test runs on $8^3 \cdot 4$ lattices near the thermodynamical cross over are given.

2 Lattice action

In this paper the domain wall fermion action is constructed according to Shamir's prescription [2]. Therefore the fermion field is defined on a five dimensional hypercubic lattice and the light chiral fermion modes are located on two boundaries of the fifth dimension. The gauge field links depend only on the coordinates of the four-dimensional space-time. The bosonic Pauli-Villars fields subtracting the heavy fermion modes are introduced as in [11].

The complete lattice action is given by

$$S = S_G[U] + S_F[\bar{\Psi}, \Psi, U] + S_{PV}[\Phi^\dagger, \Phi, U] . \quad (1)$$

Here the standard Wilson action S_G for the $SU(N_c)$ gauge field U is a sum over plaquettes

$$S_G = \beta \sum_{pl} \left(1 - \frac{1}{N_c} \text{Re Tr } U_{pl} \right) , \quad (2)$$

with the bare gauge coupling given by $\beta \equiv 2N_c/g^2$. In particular, in QCD the number of colours is $N_c = 3$. The Pauli-Villars action in (1) S_{PV} will be discussed later and the fermion action S_F for a single fermion flavour is given by

$$S_F = \sum_{x,s;x',s'} \bar{\Psi}(x', s') D_F(x', s'; x, s) \Psi(x, s) . \quad (3)$$

The four-dimensional space-time coordinates are denoted by x, x' and the fifth coordinates are s, s' . The domain wall fermion matrix D_F is constructed from the standard four-dimensional Wilson fermion matrix

$$D(x', x) = \delta_{x'x} (4 - am_0) - \frac{1}{2} \sum_{\mu=1}^4 \left[\delta_{x', x+\hat{\mu}} (1 + \gamma_\mu) U_{x\mu} + \delta_{x'+\hat{\mu}, x} (1 - \gamma_\mu) U_{x'\mu}^\dagger \right] . \quad (4)$$

The notations are standard: a is the (four-dimensional) lattice spacing and $\hat{\mu}$ denotes the unit vector in direction μ . The bare mass $-m_0$ is chosen to be negative and should be

tuned properly for producing the light boundary fermion state. In an s -block notation the domain wall fermion matrix is

$$D_F = \begin{pmatrix} \sigma + D & -\sigma P_L & 0 & 0 & \dots & 0 & 0 & am_f P_R \\ -\sigma P_R & \sigma + D & -\sigma P_L & 0 & \dots & 0 & 0 & 0 \\ 0 & -\sigma P_R & \sigma + D & -\sigma P_L & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -\sigma P_R & \sigma + D & -\sigma P_L \\ am_f P_L & 0 & 0 & 0 & \dots & 0 & -\sigma P_R & \sigma + D \end{pmatrix}. \quad (5)$$

Here m_f denotes the bare fermion mass of the light boundary fermion, $P_R = \frac{1}{2}(1 + \gamma_5)$, $P_L = \frac{1}{2}(1 - \gamma_5)$ are chiral projectors and $\sigma \equiv a/a_s$ determines the lattice spacing in the fifth dimension a_s relative to a [16].

The domain wall fermion matrix D_F is non-hermitean but it satisfies the relation

$$D_F^\dagger = \gamma_5 R_5 D_F \gamma_5 R_5 \quad (6)$$

with the reflection in the fifth dimension $(R_5)_{s',s} \equiv \delta_{s',N_s+1-s}$, ($1 \leq s \leq N_s$). This relation implies that the determinant of D_F is real and $\tilde{D}_F \equiv \gamma_5 R_5 D_F$ is hermitean. Using the hermitean Wilson fermion matrix $\tilde{D} \equiv \gamma_5 D$ the hermiticity of \tilde{D}_F is nicely displayed in an s -block form:

$$\tilde{D}_F = \begin{pmatrix} -am_f P_L & 0 & 0 & \dots & 0 & 0 & -\sigma P_R & \sigma \gamma_5 + \tilde{D} \\ 0 & 0 & 0 & \dots & 0 & -\sigma P_R & \sigma \gamma_5 + \tilde{D} & \sigma P_L \\ 0 & 0 & 0 & \dots & -\sigma P_R & \sigma \gamma_5 + \tilde{D} & \sigma P_L & 0 \\ 0 & 0 & 0 & \dots & \sigma \gamma_5 + \tilde{D} & \sigma P_L & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ -\sigma P_R & \sigma \gamma_5 + \tilde{D} & \sigma P_L & \dots & 0 & 0 & 0 & 0 \\ \sigma \gamma_5 + \tilde{D} & \sigma P_L & 0 & \dots & 0 & 0 & 0 & am_f P_R \end{pmatrix}. \quad (7)$$

The Pauli-Villars action is designed to cancel the contribution of the heavy fermions in the large N_s limit. It has a Gaussian form resulting after integration in the inverse of the fermion determinant. In order that the Gaussian integrals be well defined let us first

only consider the case of two degenerate fermion flavours when the Pauli-Villars action is

$$S_{PV} = \sum_{x,s;x',s';x'',s''} \Phi^\dagger(x'',s'') D_F^\dagger(x'',s'';x',s')_{am_f=1} D_F(x',s';x,s)_{am_f=1} \Phi(x,s) . \quad (8)$$

As it is shown by the notation, the bare mass parameter am_f is fixed here at $am_f = 1$. After performing the Grassmannian integrals over the fermion fields $\bar{\Psi}, \Psi$ and the Gaussian integrals over the Pauli-Villars fields Φ^\dagger, Φ the result, for two degenerate fermion flavours, is the ratio of determinants

$$\frac{\det(D_F) \det(D_F)}{\det(D_{F,am_f=1}^\dagger D_{F,am_f=1})} = \frac{\det(\tilde{D}_F^2)}{\det(\tilde{D}_{F,am_f=1}^2)} . \quad (9)$$

Here we used the fact that $\det(D_F)$ is real and $\det(D_F) = \det(\tilde{D}_F)$.

According to (9) the effective gauge action describing two degenerate flavours of fermions is a function of the squared hermitean fermion matrix \tilde{D}_F^2 . The same is also true in case of any number of flavours, as it will be discussed in the next section. The non-zero matrix elements of \tilde{D}_F^2 are, in an s -block form:

$$\begin{aligned} (\tilde{D}_F^2)_{s,s} &= 2\sigma^2 + 2\sigma D_r + \tilde{D}^2 + \delta_{s,1}(a^2 m_f^2 - \sigma^2)P_L + \delta_{s,N_s}(a^2 m_f^2 - \sigma^2)P_R , \\ (\tilde{D}_F^2)_{s,s+1} &= (\tilde{D}_F^2)_{s+1,s} = -\sigma^2 - \sigma D_r , \\ (\tilde{D}_F^2)_{1,N_s} &= (\tilde{D}_F^2)_{N_s,1} = am_f(\sigma + D_r) , \end{aligned} \quad (10)$$

where $D_r = \frac{1}{2}(\gamma_5 \tilde{D} + \tilde{D} \gamma_5)$ contains the Wilson term in the Wilson-fermion action:

$$D_r(x',x) = \delta_{x'x} (4 - am_0) - \frac{1}{2} \sum_{\mu=1}^4 \left[\delta_{x',x+\hat{\mu}} U_{x\mu} + \delta_{x'+\hat{\mu},x} U_{x'\mu}^\dagger \right] . \quad (11)$$

3 TSMB algorithm for domain wall fermions

The absolute value of the fermion determinant of an arbitrary (integer) number N_f of domain wall fermion flavours is, according to (9),

$$\left| \det(\tilde{D}_F) \right|^{N_f} = \left\{ \det(\tilde{D}_F^2) \right\}^{N_f/2} . \quad (12)$$

Negative values of N_f describe the Pauli-Villars fields. (The mass parameter am_f is different for physical fermion flavours and for Pauli-Villars fields, but this difference does not play a rôle in what follows.) For odd numbers of flavours the sign of the determinant is neglected in (12). However, if the mass parameter is positive ($m_f > 0$) this sign

is expected to be irrelevant because of the relation of domain wall fermions to overlap fermions which have a positive determinant if the mass is positive [17, 4].

Multi-boson algorithms [18] are based on polynomial approximations P_n satisfying

$$\lim_{n \rightarrow \infty} P_n(x) = x^{-N_f/2} \quad (13)$$

which allow to represent the fermion determinant as

$$\left\{ \det(\tilde{D}_F^2) \right\}^{N_f/2} \simeq \frac{1}{\det P_n(\tilde{D}_F^2)} . \quad (14)$$

Assuming that the polynomial roots occur in complex conjugate pairs, one can write P_n as

$$P_n(\tilde{D}_F^2) \propto \prod_{j=1}^n (\tilde{D}_F - \rho_j^*)(\tilde{D}_F - \rho_j) . \quad (15)$$

This leads to the *multi-boson representation*

$$\begin{aligned} \left| \det(\tilde{D}_F) \right|^{N_f} &\propto \prod_{j=1}^n \det[(\tilde{D}_F - \rho_j^*)(\tilde{D}_F - \rho_j)]^{-1} \\ &\propto \int [d\phi][d\phi^\dagger] \exp \left\{ - \sum_{j=1}^n \sum_{xx'} \phi_{jx'}^\dagger [(\tilde{D}_F - \rho_j^*)(\tilde{D}_F - \rho_j)]_{x'x} \phi_{jx} \right\} . \end{aligned} \quad (16)$$

Here ϕ_{jx} , ($j = 1, 2, \dots, n$) are complex boson (pseudofermion) fields.

The two-step multi-boson algorithm [15] is based, instead of (13), on a polynomial approximation by a product of polynomials

$$\lim_{n_2 \rightarrow \infty} P_{n_1}^{(1)}(x) P_{n_2}^{(2)}(x) = x^{-N_f/2} , \quad (17)$$

where the first polynomial $P_{n_1}^{(1)}(x)$ itself is an approximation to $x^{-N_f/2}$, but it has a relatively low order. The multi-boson representation (16) is only used for the first polynomial $P_{n_1}^{(1)}$. The correction factor $P_{n_2}^{(2)}$ in

$$\left| \det(\tilde{D}_F) \right|^{N_f} \simeq \frac{1}{\det P_{n_1}^{(1)}(\tilde{D}_F^2) \det P_{n_2}^{(2)}(\tilde{D}_F^2)} \quad (18)$$

is realized in a stochastic *noisy Metropolis correction step* with a global accept-reject condition, in the spirit of [19]. In order to obtain the appropriate Gaussian vector for the noisy correction the inverse square root of $P_{n_2}^{(2)}$ is also needed. This can be represented by another polynomial approximation

$$P_{n_3}^{(3)}(x) \simeq P_{n_2}^{(2)}(x)^{-\frac{1}{2}} . \quad (19)$$

A practical way to obtain $P^{(3)}$ is to use a Newton iteration

$$P_{k+1}^{(3)} = \frac{1}{2} \left(P_k^{(3)} + \frac{1}{P_k^{(3)} P^{(2)}} \right), \quad k = 0, 1, 2, \dots \quad (20)$$

The TSMB algorithm becomes exact only in the limit of infinitely high polynomial order: $n_2 \rightarrow \infty$ in (17)-(18). Instead of investigating the dependence of expectation values on n_2 by performing several simulations, it is better to fix some relatively high order n_2 for the simulation and perform another correction in the “measurement” of expectation values by still finer polynomials. This is done by *reweighting* the configurations [20]. The reweighting for general N_f is based on a polynomial approximation $P_{n_4}^{(4)}$ which satisfies

$$\lim_{n_4 \rightarrow \infty} P_{n_1}^{(1)}(x) P_{n_2}^{(2)}(x) P_{n_4}^{(4)}(x) = x^{-N_f/2}. \quad (21)$$

For more details see, for instance, [21, 22].

Up to this point the particular form of the domain wall fermion action introduced in the previous section makes no difference compared to other applications of TSMB. The occurrence of negative number of flavours, as used for the Pauli-Villars fields, is the only new feature. However, for even number of flavours one can just use the form given by (9). In this case the first polynomial $P^{(1)}$ for the Pauli-Villars fields is exact and no corrections are needed. For odd number of flavours one has to deal with polynomial approximations of some integer power of \sqrt{x} and the machinery of polynomial approximations works as usual.

Another peculiarity of domain wall fermions is that the fermion field has an extra index labeling the fifth coordinate. In practice this can easily lead to a situation where the storage of n_1 multi-boson fields in computer memory becomes a problem. (For typical simulation parameters including the values of n_1 see the recent studies in [23, 24, 25].) Fortunately, in cases if the storage of the multi-boson fields is problematic, one can organize the gauge field update in such a way that the dependence on the multi-boson fields is collected in a few auxiliary $3 \otimes 3$ matrix fields which can be easily stored in memory. The multi-boson fields can be kept on disk and have to be read before and written back after a complete boson field update. The duration of the input-output is negligible compared to the time of the update.

The auxiliary $3 \otimes 3$ matrix fields are spin-traces over the multi-boson fields which can be constructed as follows. The dependence of the effective gauge field action on the multi-boson fields can be summarized by the formula

$$S_{eff}(U_{x\mu}, \phi) = \text{Re Tr} \left(U_{x\mu} S_{x\mu}^{(1)}(\phi) + U_{x\mu} S_{x\mu}^{(2)}(\phi) \right) + \dots \quad (22)$$

Here $U_{x\mu}$ is the gauge link variable to be updated. The omitted part denoted by the dots contain terms from the pure gauge action and other terms which do not depend on $U_{x\mu}$. $S_{x\mu}^{(1,2)}(\phi)$ display the dependence on the multi-boson fields. $S^{(1)}$ gives the nearest neighbour contributions and $S^{(2)}$, which appears because of the quadratic nature of \tilde{D}_F^2 , stands for next-to-nearest neighbour contributions. A consideration of the multi-boson action (16) and of the matrices in (7), (10) gives that

$$S_{x\mu}^{(1)}(\phi) = \sum_{s=1}^{N_s} \left(\tilde{f}_{s,N_s+1-s;x\mu} + \chi f_{s,s;x\mu}^{(r)} \right) + \mu_f f_{1,N_s;x\mu}^{(r)} - \sigma \sum_{s=1}^{N_s-1} f_{s,s+1;x\mu}^{(r)} \quad (23)$$

and

$$S_{x\mu}^{(2)}(\phi) = \sum_{\nu \neq \mu, \nu=1}^4 \left(f_{x,\mu\nu}^{(++)} U_{x+\hat{\mu},\nu} + f_{x,\mu\nu}^{(+-)} U_{x+\hat{\mu}-\hat{\nu},\nu}^\dagger + U_{x,\nu}^\dagger f_{x+\hat{\nu},\nu\mu}^{(-+)} + U_{x-\hat{\nu},\nu} f_{x-\hat{\nu},\nu\mu}^{(++)} \right) . \quad (24)$$

Here we used the notations

$$\mu_f \equiv am_f , \quad \mu_0 \equiv am_0 , \quad \chi \equiv 4 - \mu_0 + \sigma . \quad (25)$$

The traces over spinor indices appearing in (23), resp. (24) are defined as

$$\begin{aligned} \tilde{f}_{s',s;x\mu} &\equiv - \sum_{j=1}^{n_1} \text{Re } \rho_j \text{Tr}_{\text{sp}} \left[(\gamma_5 + \gamma_5 \gamma_\mu) \phi_{js,x} \phi_{js',x+\hat{\mu}}^\dagger \right] + (s \leftrightarrow s') , \\ f_{s',s;x\mu}^{(r)} &\equiv - \sum_{j=1}^{n_1} \text{Tr}_{\text{sp}} \left[\phi_{js,x} \phi_{js',x+\hat{\mu}}^\dagger \right] + (s \leftrightarrow s') , \\ f_{x,\mu\nu}^{(++)} &\equiv \frac{1}{2} \sum_{j=1}^{n_1} \sum_{s=1}^{N_s} \text{Tr}_{\text{sp}} \left[(1 + \gamma_\mu - \gamma_\nu - \gamma_\nu \gamma_\mu) \phi_{js,x} \phi_{js,x+\hat{\mu}+\hat{\nu}}^\dagger \right] , \\ f_{x,\mu\nu}^{(+-)} &\equiv \frac{1}{2} \sum_{j=1}^{n_1} \sum_{s=1}^{N_s} \text{Tr}_{\text{sp}} \left[(1 + \gamma_\mu + \gamma_\nu + \gamma_\nu \gamma_\mu) \phi_{js,x} \phi_{js,x+\hat{\mu}-\hat{\nu}}^\dagger \right] , \\ f_{x,\nu\mu}^{(-+)} &\equiv \frac{1}{2} \sum_{j=1}^{n_1} \sum_{s=1}^{N_s} \text{Tr}_{\text{sp}} \left[(1 - \gamma_\nu - \gamma_\mu + \gamma_\nu \gamma_\mu) \phi_{js,x} \phi_{js,x-\hat{\nu}+\hat{\mu}}^\dagger \right] . \end{aligned} \quad (26)$$

The indices on the multi-boson fields $\phi_{js,x}$ are as follows: j is labeling the different multi-boson fields as they appear in (16), x is the four-dimensional site and s the fifth coordinate. The colour and spinor indices are not shown. After performing the trace over spinor indices the result is, of course, a $3 \otimes 3$ complex matrix.

Using the formulas (23)-(26) the effect of the multi-boson fields can be collected in the auxiliary $3 \otimes 3$ matrices. The total number of $3 \otimes 3$ matrices to be stored in memory is

$4 + 3 \cdot 12 = 40$ per four-dimensional site, which is usually not a problem. The multi-boson fields can be updated one-by-one and kept otherwise on disk. This means that one has to store $\phi_{js,x}$ only for a single value of the multi-boson index j . Of course, due to the index s , the storage requirement is increasing with N_s .

4 Numerical simulation tests

Test runs have been performed for two degenerate quark flavours $N_f = 2$ on $8^3 \cdot 4$ lattices in the vicinity of the $N_t = 4$ thermodynamic crossover. The parameter sets have been chosen from the points in parameter space which were investigated in [12]. Typical parameters were: $\mu_0 = 1.9$, $\mu_f = 0.1$, $\sigma = 1.0, 0.5$ and $5.20 \leq \beta \leq 5.45$.

The first task is to determine the parameters of the necessary polynomials for different extensions of the fifth dimension N_s . These will be largely influenced by the condition number of the squared hermitean fermion matrix \tilde{D}_F^2 , because the interval $[\epsilon, \lambda]$ where the polynomial approximations are optimized has to cover the eigenvalues of \tilde{D}_F^2 on a typical gauge configuration. A set of polynomial parameters for different N_s is given in table 1. As it is shown by the table, the largest eigenvalues of \tilde{D}_F^2 are only slightly increasing with N_s but, in the covered range, the smallest ones decrease roughly proportional to $1/N_s$. Therefore the condition number λ/ϵ is proportional to N_s . (For a discussion of bounds on the condition number see [26].)

Table 1: *Parameters of the polynomials used on $8^3 \cdot 4$ lattice for different lattice spacings and extensions of the fifth dimension. The bare parameters in the lattice action are specified in the text. The last column shows the average number of inverter iterations in the quasi heatbath update step.*

σ	N_s	n_1	n_2	n_3	n_4	ϵ	λ	I_{QHB}
1.0	8	44	240	300	300	0.011	56.0	5000
1.0	12	56	300	450	470	0.0071	57.0	7900
1.0	16	64	350	470	500	0.0052	58.0	9700
1.0	24	72	450	640	640	0.0032	59.0	12300
0.5	6	48	270	350	360	0.0071	43.0	6000
0.5	12	64	400	570	570	0.0046	44.0	10100

Table 1 refers to the case $N_f = 2$ which is considered in the present paper. As

discussed in the previous section, an odd number of flavours would also require polynomial approximations for the Pauli-Villars fields. Since the mass parameter is kept there at $\mu_f = 1$, the corresponding condition numbers are much smaller and the polynomial orders substantially lower. In the runs shown by table 1 the ratio of condition numbers is typically of the order of 10. This would require, for instance, in case of the first line of the table polynomial orders $n_1 = 32$, $n_2 = 60$, $n_3 = 90$, $n_4 = 100$.

A first estimate of the computation work can be given in terms of the number of fermion-matrix vector multiplications needed for performing a sweep over the multi-boson and gauge fields. An approximate formula per update cycles is:

$$N_{MVM} \simeq 2I_{QHB}c_{QHB}^{-1} + 6(n_1N_B + N_G) + 2N_C(n_2 + n_3) . \quad (27)$$

Here N_B is the number of boson field update sweeps per cycle, N_G the number of gauge field update sweeps and N_C the number of noisy Metropolis accept-reject steps. It is assumed that a global quasi heatbath for the boson fields [27] is performed once per c_{QHB} cycles with a average number of matrix inverter iterations I_{QHB} . (Note that I_{QHB} is a sum over n_1 inversions.) The relative contributions of the three terms in (27) are subject to optimization. The quasi heatbath is typically an important part of operations and I_{QHB} is characteristic for the total number of matrix vector multiplications N_{MVM} . For the actual values occurring in the runs see table 1 which shows that, for a given value of lattice spacing ratio σ , I_{QHB} increases somewhat faster than $N_s^{\frac{1}{2}}$.

In order to obtain an estimate for the total amount of necessary computation work, N_{MVM} has to be multiplied by the integrated autocorrelation length τ_{int} given in number of update cycles. The measurement of autocorrelations requires high statistics and a lot of computer time and is beyond the scope of the present paper. A rough estimate based on previous experience with TSMB tells that τ_{int} is proportional to n_1 . According to the table a very rough estimate for the increase of n_1 is $n_1 \propto N_s^{\frac{1}{2}}$. Taking into account that a single matrix vector multiplication grows linearly with N_s , this would finally imply that the increase of the necessary computation work is between $\propto N_s^2$ and $\propto N_s^3$. The fast increase with N_s favors domain wall fermion schemes with $\sigma < 1$ and relatively small N_s , as proposed in [28].

As these test runs show, the application of the TSMB algorithm for numerical simulations of domain wall quarks is possible. Simulations using alternative formulations based on overlap fermions, as proposed in [26], should also be feasible along the same lines. The interesting question about the computation speed compared to, say, Wilson quarks requires a more detailed analysis including the measurement of autocorrelations. Since the good chiral properties of domain wall fermions develop only sufficiently close to the

continuum limit, the performance studies have to be finally performed on large lattices.

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